



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 06:16 AM GMT

PDB ID : 4L39
Title : Crystal structure of GH3.12 from Arabidopsis thaliana in complex with AM-PCPP and salicylate
Authors : Zubietta, C.; Jez, J.M.; Brown, E.; Marcellin, R.; Kapp, U.; Round, A.; Westfall, C.
Deposited on : 2013-06-05
Resolution : 2.81 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

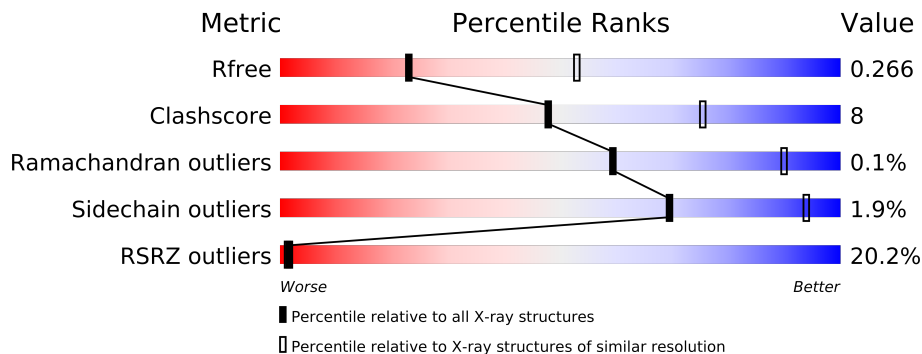
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



The reported resolution of this entry is 2.81 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1963 (2.84-2.80)
Clashscore	79885	2478 (2.84-2.80)
Ramachandran outliers	78287	2429 (2.84-2.80)
Sidechain outliers	78261	2431 (2.84-2.80)
RSRZ outliers	66119	1966 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	581	
1	B	581	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SAL	A	602	-	X
3	SAL	B	601	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8660 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 4-substituted benzoates-glutamate ligase GH3.12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	7	0
			4153	2637	681	807	28			
1	B	542	Total	C	N	O	S	0	6	0
			4211	2672	681	831	27			

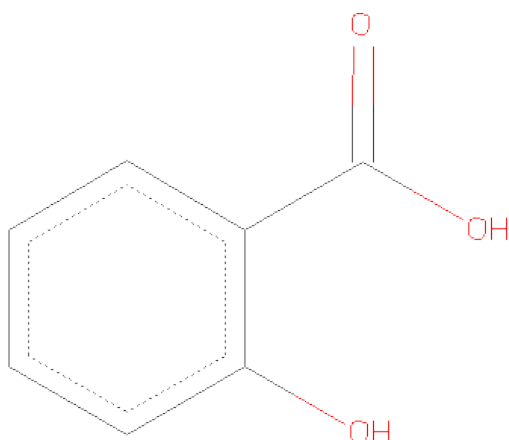
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	EXPRESSION TAG	UNP Q9LYU4
A	-4	SER	-	EXPRESSION TAG	UNP Q9LYU4
A	-3	HIS	-	EXPRESSION TAG	UNP Q9LYU4
A	-2	MET	-	EXPRESSION TAG	UNP Q9LYU4
A	-1	ALA	-	EXPRESSION TAG	UNP Q9LYU4
A	0	SER	-	EXPRESSION TAG	UNP Q9LYU4
B	-5	GLY	-	EXPRESSION TAG	UNP Q9LYU4
B	-4	SER	-	EXPRESSION TAG	UNP Q9LYU4
B	-3	HIS	-	EXPRESSION TAG	UNP Q9LYU4
B	-2	MET	-	EXPRESSION TAG	UNP Q9LYU4
B	-1	ALA	-	EXPRESSION TAG	UNP Q9LYU4
B	0	SER	-	EXPRESSION TAG	UNP Q9LYU4

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

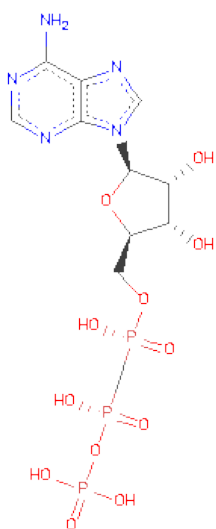
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: C₇H₆O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	7	3		
3	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 4 is DIPHOSPHOMETHYLPHOSPHONICACID ADENOSYL ESTER (three-letter code: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 5 is water.

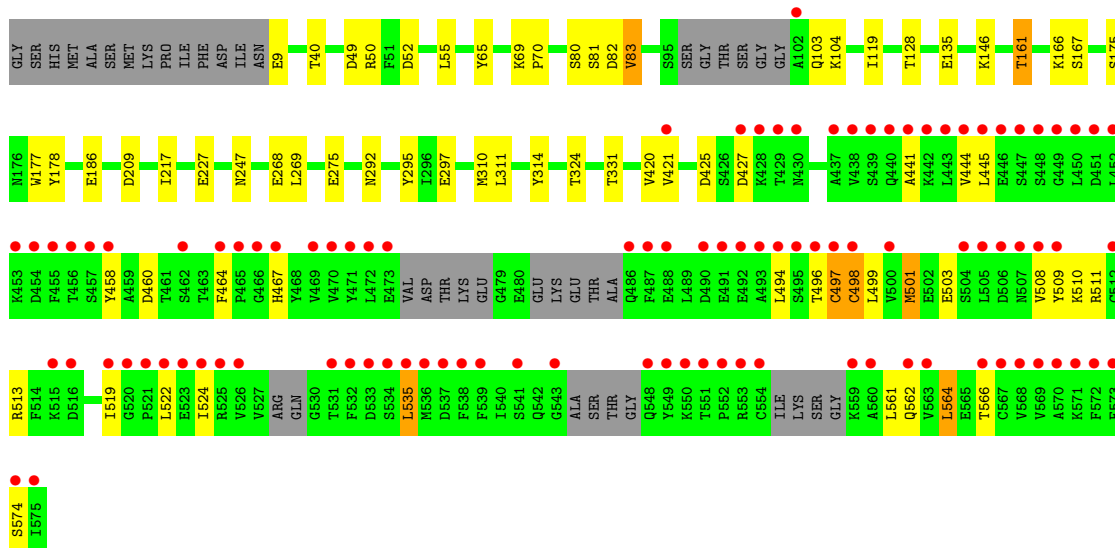
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	106	Total	O	0	0
			106	106		
5	B	107	Total	O	0	0
			107	107		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

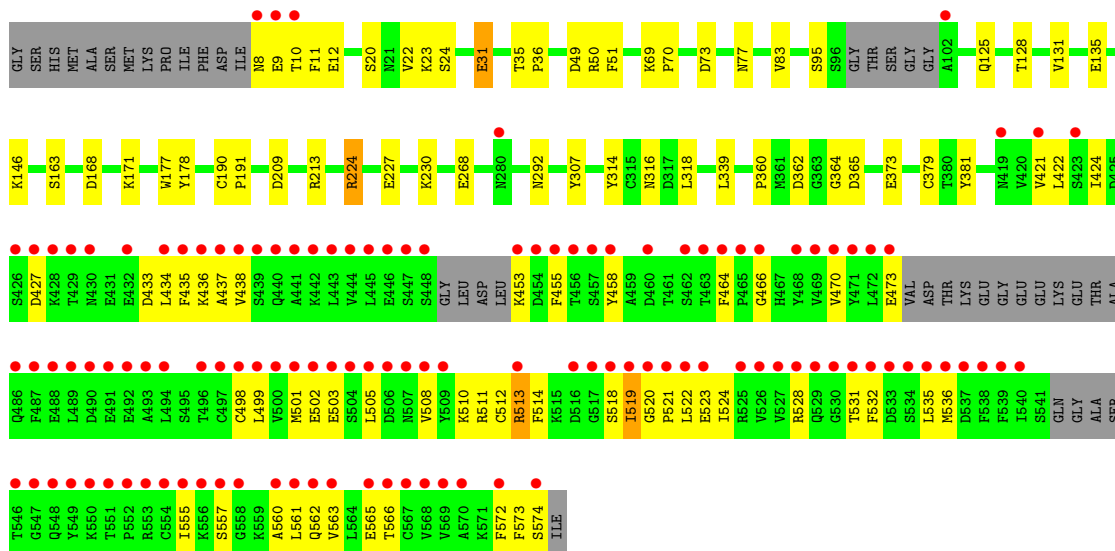
- Molecule 1: 4-substituted benzoates-glutamate ligase GH3.12

Chain A: 



- Molecule 1: 4-substituted benzoates-glutamate ligase GH3.12

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.36Å 114.09Å 157.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.00 – 2.81 58.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.00-2.81) 99.8 (58.00-2.81)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	0.26	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1391)	Depositor
R, R_{free}	0.198 , 0.267 0.197 , 0.266	Depositor DCC
R_{free} test set	1416 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 25.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 28176 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8660	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.16 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.7619e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: APC, MG, SAL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.78	2/4251 (0.0%)	0.77	1/5770 (0.0%)
1	B	0.78	0/4309	0.78	2/5850 (0.0%)
All	All	0.78	2/8560 (0.0%)	0.77	3/11620 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	497	CYS	CB-SG	-6.99	1.70	1.82
1	A	275	GLU	CB-CG	-6.16	1.40	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	513	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	564	LEU	CB-CG-CD2	-5.33	101.94	111.00
1	B	224	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	520	GLY	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4153	0	3910	51	0
1	B	4211	0	4003	79	0
2	A	1	0	0	0	0
3	A	10	0	5	0	0
3	B	10	0	5	0	0
4	A	31	0	14	1	0
4	B	31	0	14	0	0
5	A	106	0	0	2	0
5	B	107	0	0	6	0
All	All	8660	0	7951	130	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (130) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:310:MET:HE2	1:A:314:TYR:CZ	2.10	0.86
1:B:512:CYS:HG	1:B:518:SER:HG	1.15	0.84
1:B:8:ASN:N	5:B:739:HOH:O	2.12	0.82
1:B:513:ARG:NH2	1:B:521:PRO:HA	1.95	0.81
1:A:562:GLN:O	1:A:566:THR:HG23	1.84	0.77
1:A:535:LEU:HD13	1:A:564:LEU:HD21	1.67	0.75
1:B:427:ASP:HA	1:B:508:VAL:HG11	1.69	0.72
1:B:513:ARG:HD3	1:B:519:ILE:HB	1.74	0.69
1:A:310:MET:CE	1:A:314:TYR:CZ	2.74	0.69
1:A:501:MET:HE2	1:A:522:LEU:HD21	1.72	0.69
1:B:31:GLU:HG2	1:B:51:PHE:CE2	2.28	0.68
1:B:453:LYS:N	1:B:473:GLU:O	2.29	0.66
1:A:65:TYR:CE1	1:A:104:LYS:HD2	2.31	0.66
1:B:49:ASP:OD1	1:B:50:ARG:NH1	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:562:GLN:O	1:B:566:THR:OG1	2.09	0.65
1:A:80:SER:O	1:A:83:VAL:HG13	1.97	0.64
1:B:499:LEU:HD23	1:B:502:GLU:HG3	1.79	0.64
1:B:20:SER:O	5:B:718:HOH:O	2.14	0.64
1:A:445:LEU:HD11	1:A:497:CYS:SG	2.38	0.64
1:B:268:GLU:OE2	5:B:774:HOH:O	2.14	0.63
1:B:532:PHE:HA	1:B:535:LEU:HB3	1.80	0.62
1:A:501:MET:CE	1:A:522:LEU:HD21	2.29	0.62
1:B:437:ALA:HB1	1:B:501:MET:HG2	1.81	0.61
1:B:513:ARG:HH11	1:B:519:ILE:HB	1.67	0.60
1:A:310:MET:HE2	1:A:314:TYR:CE2	2.37	0.59
1:B:512:CYS:SG	1:B:518:SER:OG	2.42	0.58
1:B:522:LEU:HD12	1:B:523:GLU:N	2.19	0.58
1:B:427:ASP:HB3	1:B:508:VAL:HG12	1.85	0.58
1:A:227:GLU:HG3	1:A:464:PHE:CG	2.38	0.58
1:A:146:LYS:HZ1	1:A:511:ARG:HD2	1.68	0.58
1:B:12:GLU:N	1:B:12:GLU:OE1	2.37	0.58
1:B:470:VAL:HG23	1:B:522:LEU:HD11	1.86	0.57
1:B:421:VAL:HG23	1:B:422:LEU:HD12	1.85	0.57
1:B:499:LEU:HD23	1:B:502:GLU:CG	2.35	0.57
1:A:445:LEU:CD1	1:A:497:CYS:SG	2.93	0.56
1:B:513:ARG:NH1	1:B:519:ILE:HG22	2.20	0.56
1:B:35:THR:O	5:B:738:HOH:O	2.17	0.55
1:A:513:ARG:HA	1:A:519:ILE:HB	1.88	0.55
1:B:513:ARG:HH22	1:B:521:PRO:HA	1.68	0.55
1:B:178:TYR:O	1:B:213:ARG:NH2	2.41	0.54
1:B:499:LEU:CD2	1:B:502:GLU:HG3	2.37	0.54
1:B:458:TYR:CE1	1:B:561:LEU:HD11	2.43	0.53
1:B:373:GLU:N	1:B:373:GLU:OE1	2.41	0.53
1:A:501:MET:HE2	1:A:522:LEU:CD2	2.40	0.52
1:B:513:ARG:HH11	1:B:519:ILE:CB	2.22	0.52
1:B:427:ASP:HA	1:B:508:VAL:CG1	2.38	0.52
1:A:268[A]:GLU:HG2	1:A:269:LEU:N	2.25	0.52
1:A:535:LEU:HD12	1:A:564:LEU:HD11	1.92	0.51
1:B:23:LYS:HD3	1:B:373:GLU:HG3	1.93	0.51
1:B:131:VAL:HG22	1:B:339:LEU:HD21	1.93	0.51
1:B:511:ARG:HG3	1:B:512:CYS:N	2.26	0.50
1:A:161:THR:HG21	1:A:217:ILE:HD11	1.94	0.50
1:B:22:VAL:N	5:B:718:HOH:O	2.44	0.50
1:B:23:LYS:HD2	1:B:373:GLU:OE2	2.11	0.50
1:B:307:TYR:OH	1:B:424:ILE:O	2.23	0.49
1:A:103:GLN:OE1	1:A:508:VAL:HG12	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:458:TYR:CE1	1:B:561:LEU:CD1	2.96	0.48
1:A:427:ASP:CB	1:A:509:TYR:HA	2.43	0.48
1:A:441:ALA:O	1:A:444:VAL:HG22	2.14	0.48
1:A:460:ASP:OD1	1:A:467:HIS:N	2.45	0.48
1:B:435:PHE:HA	1:B:438:VAL:HG22	1.95	0.47
1:B:560:ALA:O	1:B:563:VAL:HG22	2.13	0.47
1:B:557:SER:O	1:B:561:LEU:HD13	2.15	0.47
1:B:532:PHE:O	1:B:536:MET:N	2.47	0.47
1:B:528:ARG:N	1:B:531:THR:OG1	2.47	0.47
1:B:501:MET:O	1:B:505:LEU:HD13	2.14	0.46
1:B:73:ASP:O	1:B:77:ASN:ND2	2.48	0.46
1:B:9:GLU:C	1:B:11:PHE:H	2.17	0.46
1:B:230:LYS:NZ	1:B:314:TYR:OH	2.46	0.46
1:A:166:LYS:HA	1:A:166:LYS:HD2	1.81	0.46
1:A:247:ASN:ND2	5:A:762:HOH:O	2.46	0.46
1:A:119:ILE:HG13	1:A:331:THR:HG21	1.98	0.46
1:A:458:TYR:CE1	1:A:561:LEU:HD11	2.50	0.46
1:B:318:LEU:O	5:B:736:HOH:O	2.21	0.46
1:A:9:GLU:N	5:A:775:HOH:O	2.48	0.46
1:A:498:CYS:HB2	1:A:574:SER:HB3	1.97	0.45
1:A:499:LEU:O	1:A:503:GLU:HG3	2.17	0.45
1:A:310:MET:CE	1:A:314:TYR:CE2	2.97	0.45
1:B:168:ASP:HA	1:B:171:LYS:HG2	1.99	0.45
1:A:499:LEU:HB3	1:A:574:SER:HB2	1.99	0.45
1:B:521:PRO:O	1:B:573:PHE:HD1	1.99	0.45
1:A:324:THR:O	4:A:603:APC:N6	2.50	0.44
1:A:498:CYS:HB3	1:A:524:ILE:HD12	1.99	0.44
1:B:360:PRO:HB3	1:B:365:ASP:HB3	1.99	0.44
1:A:494:LEU:HD12	1:A:497:CYS:SG	2.58	0.44
1:B:433:ASP:HB2	1:B:436:LYS:CE	2.48	0.44
1:B:362:ASP:OD1	1:B:364:GLY:N	2.50	0.44
1:A:209:ASP:O	1:A:292:ASN:ND2	2.46	0.44
1:A:420:VAL:HG12	1:A:421:VAL:N	2.33	0.43
1:B:35:THR:N	1:B:36:PRO:HD2	2.32	0.43
1:B:146:LYS:HD2	1:B:511:ARG:NH2	2.33	0.43
1:A:128[B]:THR:HG21	1:A:135:GLU:OE2	2.19	0.43
1:B:95:SER:O	1:B:95:SER:OG	2.28	0.43
1:B:521:PRO:HB2	1:B:574:SER:HB2	2.01	0.43
1:A:496:THR:HA	1:A:499:LEU:HG	2.00	0.43
1:B:433:ASP:CB	1:B:436:LYS:HE2	2.49	0.43
1:A:177:TRP:CG	1:A:178:TYR:N	2.87	0.43
1:A:186:GLU:OE1	1:A:186:GLU:N	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:177:TRP:CD2	1:A:178:TYR:N	2.88	0.42
1:B:503:GLU:HA	1:B:510:LYS:CE	2.49	0.42
1:A:40:THR:HA	1:A:82:ASP:O	2.19	0.42
1:A:52:ASP:HB3	1:A:55:LEU:HB3	2.01	0.42
1:B:146:LYS:HE2	1:B:511:ARG:HH22	1.85	0.42
1:A:535:LEU:O	1:A:535:LEU:HG	2.20	0.42
1:B:224:ARG:HD3	1:B:464:PHE:HZ	1.84	0.42
1:A:295:TYR:CE2	1:A:297:GLU:HB2	2.55	0.42
1:B:9:GLU:HG2	1:B:10:THR:N	2.35	0.42
1:B:227:GLU:HG3	1:B:464:PHE:CD1	2.54	0.42
1:B:498:CYS:SG	1:B:524:ILE:CD1	3.08	0.42
1:A:509:TYR:CD2	1:A:510:LYS:N	2.87	0.41
1:B:209:ASP:O	1:B:292:ASN:ND2	2.45	0.41
1:B:69:LYS:N	1:B:70:PRO:CD	2.83	0.41
1:B:135:GLU:HG2	1:B:177:TRP:CD1	2.54	0.41
1:A:535:LEU:CD1	1:A:564:LEU:HD21	2.42	0.41
1:B:523:GLU:HA	1:B:572:PHE:O	2.21	0.41
1:B:379:CYS:HB2	1:B:381:TYR:CE2	2.56	0.41
1:B:466:GLY:O	1:B:519:ILE:HG23	2.21	0.41
1:B:561:LEU:O	1:B:565:GLU:N	2.46	0.41
1:B:434:LEU:O	1:B:438:VAL:HG22	2.21	0.41
1:A:69:LYS:N	1:A:70:PRO:CD	2.84	0.41
1:A:49:ASP:OD1	1:A:50:ARG:NH1	2.54	0.41
1:B:373:GLU:H	1:B:373:GLU:CD	2.25	0.40
1:A:460:ASP:OD2	1:A:467:HIS:NE2	2.54	0.40
1:B:190:CYS:HA	1:B:191:PRO:HD3	1.98	0.40
1:A:310:MET:CE	1:A:314:TYR:CE1	3.04	0.40
1:B:8:ASN:O	1:B:12:GLU:OE1	2.38	0.40
1:B:513:ARG:HG3	1:B:514:PHE:CD1	2.57	0.40
1:B:177:TRP:CG	1:B:178:TYR:N	2.89	0.40
1:B:458:TYR:CE1	1:B:555:ILE:CB	3.05	0.40
1:B:11:PHE:HB2	1:B:125:GLN:OE1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	534/581 (92%)	506 (95%)	27 (5%)	1 (0%)	56	88
1	B	537/581 (92%)	507 (94%)	30 (6%)	0	100	100
All	All	1071/1162 (92%)	1013 (95%)	57 (5%)	1 (0%)	59	90

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	425	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	445/527 (84%)	436 (98%)	9 (2%)	68	93
1	B	465/527 (88%)	456 (98%)	9 (2%)	69	94
All	All	910/1054 (86%)	892 (98%)	18 (2%)	69	93

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	SER
1	A	83	VAL
1	A	161	THR
1	A	167	SER
1	A	175	SER
1	A	311	LEU
1	A	498	CYS
1	A	501	MET
1	A	535	LEU
1	B	24[B]	SER
1	B	31	GLU
1	B	83	VAL
1	B	128[A]	THR
1	B	128[B]	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	163	SER
1	B	316	ASN
1	B	455	PHE
1	B	519	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	SAL	A	602	-	10,10,10	1.05	0	13,13,13	1.59	4 (30%)
4	APC	A	603	2	33,33,33	2.58	10 (30%)	52,52,52	2.82	14 (26%)
3	SAL	B	601	-	10,10,10	1.09	1 (10%)	13,13,13	1.12	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	APC	B	602	-	33,33,33	2.59	9 (27%)	52,52,52	2.82	15 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAL	A	602	-	-	0/4/4/4	0/1/1/1
4	APC	A	603	2	-	0/20/38/38	0/1/3/3
3	SAL	B	601	-	-	0/4/4/4	0/1/1/1
4	APC	B	602	-	-	0/20/38/38	0/1/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	APC	PB-C3A	7.91	1.86	1.79
4	A	603	APC	PA-C3A	7.53	1.86	1.79
4	B	602	APC	PA-C3A	7.41	1.86	1.79
4	A	603	APC	PB-C3A	7.02	1.85	1.79
4	B	602	APC	O4'-C1'	6.52	1.51	1.41
4	A	603	APC	O4'-C1'	6.27	1.51	1.41
4	A	603	APC	C2'-C3'	-3.52	1.43	1.53
4	A	603	APC	C2'-C1'	-3.47	1.48	1.53
4	B	602	APC	C2'-C1'	-3.27	1.48	1.53
4	A	603	APC	C1'-N9	-2.88	1.39	1.48
4	A	603	APC	O4'-C4'	2.85	1.51	1.45
4	B	602	APC	C1'-N9	-2.78	1.40	1.48
3	B	601	SAL	O2-C2	2.48	1.41	1.36
4	B	602	APC	C2'-C3'	-2.47	1.46	1.53
4	B	602	APC	O4'-C4'	2.45	1.50	1.45
4	A	603	APC	C3'-C4'	-2.44	1.46	1.53
4	A	603	APC	C5-N7	-2.17	1.32	1.40
4	B	602	APC	C2-N3	2.16	1.36	1.32
4	A	603	APC	C2-N3	2.13	1.36	1.32
4	B	602	APC	C5-N7	-2.10	1.32	1.40

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	APC	N3-C2-N1	-12.92	117.91	128.71
4	B	602	APC	N3-C2-N1	-11.36	119.21	128.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	APC	O4'-C1'-N9	9.82	117.58	108.44
4	B	602	APC	C3'-C2'-C1'	6.18	110.59	100.91
4	A	603	APC	PA-C3A-PB	-5.57	109.61	117.62
4	A	603	APC	C4'-O4'-C1'	-5.36	103.93	109.75
4	B	602	APC	N3-C4-N9	5.31	135.01	125.43
4	A	603	APC	N3-C4-N9	5.19	134.80	125.43
4	A	603	APC	C3'-C2'-C1'	5.17	108.99	100.91
4	A	603	APC	O4'-C1'-N9	4.81	112.91	108.44
4	A	603	APC	O5'-PA-O1A	-4.15	103.86	114.21
4	B	602	APC	C2'-C1'-N9	-3.80	103.52	113.27
4	B	602	APC	PA-C3A-PB	-3.70	112.30	117.62
4	B	602	APC	C4'-O4'-C1'	-3.59	105.85	109.75
3	A	602	SAL	C2-C1-C1'	3.31	123.75	120.03
4	B	602	APC	O2B-PB-C3A	3.29	114.19	106.61
4	A	603	APC	O2A-PA-O5'	2.96	115.28	105.82
4	B	602	APC	C5-C4-N3	-2.96	119.27	125.70
4	A	603	APC	O2'-C2'-C3'	-2.86	102.54	111.83
4	B	602	APC	O5'-PA-O1A	-2.81	107.20	114.21
4	B	602	APC	O5'-PA-C3A	2.61	110.45	103.97
4	A	603	APC	C2-N3-C4	2.59	121.37	114.01
4	A	603	APC	C5'-C4'-C3'	-2.58	104.87	115.21
4	A	603	APC	C5-C4-N3	-2.57	120.11	125.70
4	B	602	APC	C2-N3-C4	2.49	121.09	114.01
3	B	601	SAL	C2-C1-C1'	2.46	122.80	120.03
4	A	603	APC	O3B-PB-O1B	-2.43	106.36	111.51
3	A	602	SAL	O2'-C1'-C1	2.39	122.60	115.47
3	A	602	SAL	C3-C2-C1	2.23	122.58	119.89
4	B	602	APC	O2A-PA-C3A	2.21	111.71	106.61
4	A	603	APC	C2-N1-C6	2.17	122.69	118.77
4	B	602	APC	C4-C5-N7	-2.16	107.67	109.52
3	A	602	SAL	O2'-C1'-O1'	-2.15	118.47	123.35
4	B	602	APC	O4'-C4'-C3'	2.08	109.39	105.17
3	B	601	SAL	O2'-C1'-C1	2.01	121.48	115.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	541/581 (93%)	0.32	100 (18%) 2 2	7, 20, 138, 155	0
1	B	542/581 (93%)	0.55	120 (22%) 1 1	6, 21, 160, 182	0
All	All	1083/1162 (93%)	0.43	220 (20%) 2 1	6, 21, 150, 182	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	546	THR	17.8
1	B	554	CYS	16.1
1	A	454	ASP	12.8
1	B	448	SER	12.7
1	B	444	VAL	12.7
1	A	444	VAL	11.3
1	B	547	GLY	10.9
1	B	548	GLN	10.6
1	B	487	PHE	10.5
1	B	445	LEU	10.0
1	A	470	VAL	9.7
1	A	575	ILE	9.5
1	B	533	ASP	9.2
1	A	525	ARG	9.1
1	B	8	ASN	9.1
1	B	537	ASP	8.9
1	B	498	CYS	8.4
1	B	509	TYR	8.2
1	A	554	CYS	8.1
1	B	457	SER	8.0
1	A	445	LEU	8.0
1	A	448	SER	7.9
1	B	552	PRO	7.7
1	A	449	GLY	7.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	551	THR	7.5
1	A	572	PHE	7.5
1	B	454	ASP	7.4
1	B	497	CYS	7.4
1	B	493	ALA	7.2
1	A	438	VAL	7.1
1	A	534	SER	7.0
1	B	538	PHE	7.0
1	B	456	THR	7.0
1	B	540	ILE	7.0
1	A	570	ALA	6.9
1	A	443	LEU	6.9
1	A	450	LEU	6.6
1	A	571	LYS	6.6
1	B	443	LEU	6.6
1	B	468	TYR	6.6
1	A	437	ALA	6.5
1	B	458	TYR	6.5
1	B	534	SER	6.4
1	B	555	ILE	6.4
1	A	487	PHE	6.4
1	B	500	VAL	6.3
1	A	551	THR	6.3
1	A	566	THR	6.2
1	B	472	LEU	6.2
1	A	441	ALA	6.2
1	B	469	VAL	6.2
1	A	533	ASP	6.1
1	A	538	PHE	6.1
1	B	490	ASP	6.1
1	B	455	PHE	6.0
1	A	493	ALA	6.0
1	A	465	PRO	5.7
1	B	447	SER	5.6
1	A	537	ASP	5.6
1	A	562	GLN	5.5
1	B	471	TYR	5.3
1	B	426	SER	5.3
1	A	457	SER	5.3
1	A	488	GLU	5.3
1	A	455	PHE	5.3
1	B	525	ARG	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	453	LYS	5.3
1	B	429	THR	5.3
1	B	446	GLU	5.2
1	B	568	VAL	5.2
1	A	466	GLY	5.2
1	A	471	TYR	5.2
1	B	518	SER	5.2
1	B	549	TYR	5.2
1	B	440	GLN	5.2
1	B	437	ALA	5.1
1	A	439	SER	5.1
1	B	572	PHE	5.1
1	A	440	GLN	5.1
1	A	469	VAL	5.1
1	A	508	VAL	5.0
1	B	442	LYS	5.0
1	B	516	ASP	5.0
1	B	519	ILE	5.0
1	B	570	ALA	5.0
1	B	427	ASP	4.9
1	A	536	MET	4.8
1	B	430	ASN	4.8
1	A	505	LEU	4.8
1	B	470	VAL	4.7
1	A	452	LEU	4.7
1	A	550	LYS	4.6
1	A	563	VAL	4.6
1	B	464	PHE	4.6
1	A	458	TYR	4.5
1	A	516	ASP	4.4
1	B	562	GLN	4.2
1	A	535	LEU	4.2
1	B	517	GLY	4.2
1	B	496	THR	4.1
1	B	507	ASN	4.1
1	A	486	GLN	4.1
1	B	501	MET	4.0
1	B	102	ALA	4.0
1	B	539	PHE	4.0
1	A	473	GLU	4.0
1	B	536	MET	4.0
1	A	456	THR	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	438	VAL	3.9
1	A	532	PHE	3.9
1	B	553	ARG	3.9
1	B	466	GLY	3.9
1	B	463	THR	3.9
1	B	532	PHE	3.8
1	A	500	VAL	3.8
1	A	553	ARG	3.8
1	B	535	LEU	3.8
1	A	567	CYS	3.8
1	A	507	ASN	3.8
1	A	524	ILE	3.8
1	A	509	TYR	3.7
1	B	505	LEU	3.7
1	A	552	PRO	3.7
1	B	560	ALA	3.7
1	B	520	GLY	3.7
1	A	506	ASP	3.6
1	A	453	LYS	3.6
1	A	491	GLU	3.6
1	A	569	VAL	3.6
1	B	563	VAL	3.6
1	A	492	GLU	3.6
1	B	489	LEU	3.5
1	B	502	GLU	3.4
1	B	473	GLU	3.4
1	B	491	GLU	3.4
1	A	548	GLN	3.4
1	B	9	GLU	3.3
1	A	447	SER	3.3
1	A	574	SER	3.3
1	A	490	ASP	3.3
1	B	558	GLY	3.3
1	A	430	ASN	3.3
1	B	522	LEU	3.2
1	A	451	ASP	3.2
1	B	441	ALA	3.2
1	A	472	LEU	3.2
1	B	499	LEU	3.2
1	A	102	ALA	3.2
1	A	520	GLY	3.1
1	B	421	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	508	VAL	3.1
1	A	498	CYS	3.1
1	A	462	SER	3.1
1	B	492	GLU	3.1
1	A	494	LEU	3.0
1	B	506	ASP	3.0
1	B	528	ARG	3.0
1	A	504	SER	3.0
1	B	530	GLY	3.0
1	B	569	VAL	3.0
1	A	512	CYS	3.0
1	A	446	GLU	3.0
1	A	521	PRO	3.0
1	A	531	THR	2.9
1	B	561	LEU	2.9
1	B	503	GLU	2.9
1	A	421	VAL	2.9
1	B	526	VAL	2.9
1	B	423	SER	2.9
1	A	539	PHE	2.9
1	A	522	LEU	2.8
1	A	519	ILE	2.8
1	A	559	LYS	2.8
1	B	488	GLU	2.8
1	B	428	LYS	2.8
1	B	436	LYS	2.8
1	B	504	SER	2.7
1	B	556	LYS	2.7
1	B	566	THR	2.7
1	B	462	SER	2.7
1	B	531	THR	2.7
1	A	495	SER	2.6
1	B	419	ASN	2.6
1	B	434	LEU	2.6
1	B	439	SER	2.6
1	B	494	LEU	2.6
1	B	435	PHE	2.6
1	B	521	PRO	2.6
1	B	565	GLU	2.5
1	A	560	ALA	2.5
1	A	568	VAL	2.5
1	B	529	GLN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	549	TYR	2.5
1	A	442	LYS	2.5
1	B	567	CYS	2.5
1	A	429	THR	2.5
1	B	527	VAL	2.5
1	A	464	PHE	2.4
1	B	465	PRO	2.4
1	A	573	PHE	2.4
1	B	513	ARG	2.4
1	A	541	SER	2.4
1	B	10	THR	2.3
1	A	497	CYS	2.3
1	A	523	GLU	2.3
1	A	515	LYS	2.2
1	A	467	HIS	2.2
1	A	428	LYS	2.2
1	A	543	GLY	2.1
1	B	280	ASN	2.1
1	B	486	GLN	2.1
1	B	523	GLU	2.1
1	B	574	SER	2.1
1	B	550	LYS	2.1
1	A	496	THR	2.0
1	A	526	VAL	2.0
1	B	557	SER	2.0
1	B	432	GLU	2.0
1	A	427	ASP	2.0
1	B	460	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SAL	B	601	10/10	0.21	4.04	35,46,51,59	0
3	SAL	A	602	10/10	0.21	2.23	17,38,46,51	0
4	APC	A	603	31/31	0.15	0.00	15,30,78,84	0
2	MG	A	601	1/1	0.12	-0.37	44,44,44,44	0
4	APC	B	602	31/31	0.13	-0.43	21,39,74,83	0

6.5 Other polymers ⓘ

There are no such residues in this entry.